Nonadiabatic Factor Accompanying Magnetic Translation of a Charged Particle

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Abstract

The quantum adiabatic theorem incorporating the Berry phase phenomenon can be characterized as a factorization of the time evolution operator into the product of a path-dependent geometric factor, a usual dynamical factor and a nonadiabatic factor that approaches the identity in the adiabatic limit. We study a case where all these factors can be constructed explicitly and where the instantaneous Hamiltonian has infinitely degenerate eigenstates associated with magnetic translation symmetry.

Magnetic translation symmetry is much discussed in the literature[1, 2, 3, 4, 5, 6, 7]. The basic example is the quantum mechanics of a charged particle moving in a two-dimensional plane perpendicular to a magnetic field, i.e. the Landau level problem. The Hamiltonian is not invariant under the ordinary translation group R^2, because it is the vector potential rather than the magnetic field that appears in the Hamiltonian. The translational symmetry of the physical situation is realized through the magnetic translation. The magnetic translation concept has been found useful in a variety of physical situations including Bloch electrons in a magnetic field[8, 9, 10, 11] where there is a lattice potential present. Even so, we believe that magnetic translation symmetry as an essential tool in solving simple dynamical systems have yet to be fully explored.

In this paper, we want to show a connection between magnetic translation symmetry and the quantum adiabatic theorem involving infinitely degenerate eigenstates. We adopt the point of view that the quantum adiabatic theorem including the Berry phase phenomenon is essentially a factorization of the time evolution operator into the product of a path-dependent geometric factor and a usual dynamical factor[12, 7]. When the change of the parameters in the Hamiltonian is not slow, there should be another factor in the time-evolution operator which represents nonadiabatic effects. Naturally, this nonadiabatic factor approaches the identity operator in a suitable adiabatic limit. We want to provide an example where all these factors can be constructed explicitly for a general parameter variation and where the instantaneous Hamiltonian has infinitely degenerate energy levels.

First, we collect some basic properties on the magnetic translation to be used later. In the usual two-dimensional Landau level problem, the kinematical momentum is $\pi_\mu = p_\mu - \frac{q}{c}A_\mu(\mathbf{x}),\ \mu = 1, 2$, where $A_\mu(\mathbf{x})$ is the vector potential in arbitary gauge. Define

$$\eta_1 = \pi_1 - \frac{qB}{c}x_2 = -\frac{qB}{c}c_2, \quad \eta_2 = \pi_2 + \frac{qB}{c}x_1 = \frac{qB}{c}c_1. \tag{1}$$

In classical mechanics, (c_1, c_2) is the center of the circular motion. In quantum mechanics, we have the following commutation relations

$$[\pi_1, \pi_2] = i\hbar qB/c, \quad [\eta_1, \eta_2] = -i\hbar qB/c, \quad [\pi_\mu, \eta_\mu] = 0. \tag{2}$$

To realize a translation $\mathbf{x} \to \mathbf{x} + \mathbf{d}(t)$, instead of using the ordinary translation operator $\exp(-ip_\mu d_\mu(t)/\hbar)$ which does not commute with π_μ and the Hamiltonian, one can choose to use the magnetic translation operator $\exp(-i\eta_\mu d_\mu(t)/\hbar)$. Note that a distinction between $\exp(-i\eta_\mu d_\mu(t)/\hbar)$ and $P\exp(-i\eta_\mu d_\mu(t)/\hbar)$ has to be made because η_1 and η_2 do not commute. Let

$$P\exp(-i\eta_\mu d_\mu(t)/\hbar) = e^{i\beta(C(\mathbf{d}))}\exp(-i\eta_\mu d_\mu(t)/\hbar). \tag{3}$$

Then the phase $\beta(C(\mathbf{d}))$ is determined by the path C traversed by $\mathbf{d}(t)$. In particular, for a closed path, $\beta(C(\mathbf{d}))$ is equal to $-\frac{q\phi}{\hbar c}$, where ϕ is the magnetic flux enclosed by the loop of C. One can similarly consider path-ordered or time-ordered operators generated by π_μ. The magnetic translation group is defined by Zak as the set of path-ordered magnetic translation operators[2, 3].

Now let us consider a charged particle moving in a two-dimensional plane with $\mathbf{x} = (x_1, x_2)$ whose Hamiltonian depends on a parameter $\mathbf{R}(t) = (R_1(t), R_2(t))$:

$$H_L = \frac{1}{2m}\big[\mathbf{p} - \frac{q}{c}\mathbf{A}_L(x, \mathbf{R})\big]^2, \tag{4}$$

where

$$\mathbf{A}_L(x, \mathbf{R}) = \frac{B}{2}\mathbf{e}_3 \times \big[\mathbf{x} - \mathbf{R}(t)\big]. \tag{5}$$

The Hamiltonian H_L for a fixed $\mathbf{R}$ is just a Landau level Hamiltonian with the magnetic field direction $\mathbf{e}_3$ perpendicular to the (x_1, x_2) plane. Our purpose is to study the case when $\mathbf{R}(t)$ varies with time.

Now a crude estimation of how the wave packet moves. The vector potential, in addition to the uniform magnetic field in the $\mathbf{e}_3$ direction, represents an electric field $\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} = \frac{B}{2c}\mathbf{e}_3 \times \dot{\mathbf{R}}(t)$. To balance out this electric field, the charged particle may generate a Lorentz force with a velocity $\dot{\mathbf{R}}(t)/2$. Therefore it makes sense to conjecture that the wave packet is shifted by $(\mathbf{R}(t) - \mathbf{R}(0))/2$ at time t instead of $\mathbf{R}(t) - \mathbf{R}(0)$. This picture should be correct at least for the special case of a constant electric field which is a well understood example in quantum mechanics. There has also been study of the special case when the electric field is along a fixed direction and is time-dependent[13]. Our purpose here is to examine the general case with the magnetic translation concept as an essential tool and to provide a rigorous demonstration of the quantum adiabatic theorem involving infinitely degenerate energy levels.

With the above physical picture, it is reasonable to resist any temptation to believe that a wave packet initially centered at $\mathbf{R}(0)$ will be displaced to be centered at point $\mathbf{R}(t)$ at time t, almost as one should resist a temptation to believe that the wave packet is not being displaced at all and it's just the wavefunction that undergoes a time dependent local gauge transformation that has no observable consequence. These two contradicting scenarios have one thing in common: They can transform an eigenfunction of the initial Hamiltonian to an instantaneous eigenfunction of $H_L(t)$. Yet there are infinitely many transformations that can achieve the same goal. Consider the local gauge transformation scenario in which the initial eigenstate is not displaced but is gauge transformed to be an instantaneous eigenstate. One might perform a magnetic translation first before doing the gauge transformation. In this paper we show that, under this layer of local gauge transformation that depends on the value of $\mathbf{R}(t)$, the motion of a wave packet is described by a path-ordered magnetic translation corresponding to the displacement $(\mathbf{R}(t) - \mathbf{R}(0))/2$ and this path-ordered magnetic translation is accompanied by a nonadiabatic operator that depends on the rate of change of $\mathbf{R}(t)$. This nonadiabatic operator is explicitly constructed for general parameter variation.

The Schrödinger equation that corresponds to H_L is

$$i\hbar\frac{\partial}{\partial t}\Psi_L(\mathbf{x}, t) = H_L\Psi_L(\mathbf{x}, t). \tag{6}$$

Now consider the gauge transformation

$$\Psi_L(\mathbf{x},t) = \exp[-i\frac{q}{\hbar c}\chi(\mathbf{x},t)]\Psi(\mathbf{x},t), \tag{7}$$

where

$$\chi(\mathbf{x},t) = -\frac{B}{2}(R_2(t)-R_2(0))x_1 + \frac{B}{2}(R_1(t)-R_1(0))x_2. \tag{8}$$

Then $\Psi(\mathbf{x},t)$ can be shown to satisfy the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t) = H\Psi(\mathbf{x},t), \tag{9}$$

where

$$H = \frac{1}{2m}\big[\mathbf{p} - \frac{q}{c}\mathbf{A}(\mathbf{x})\big]^2 - \frac{q}{c}\frac{\partial}{\partial t}\chi(\mathbf{x},t), \tag{10}$$

$$\mathbf{A}(\mathbf{x}) = \frac{B}{2}\mathbf{e}_3 \times \big[\mathbf{x} - \mathbf{R}(0)\big]. \tag{11}$$

This particular gauge transformation, the one we mentioned earlier that transforms any initial eigenfunction to an instantaneous eigenfunction, induces a transformation between the time evolution operators:

$$U_L(t,0) = \exp[-i\frac{q}{\hbar c}\chi(\mathbf{x},t)]U(t,0). \tag{12}$$

Our goal is to find the factorization of $U(t,0)$ corresponding to H into the product of three factors, each of them has a distinct physical meaning. From such a factorization, the structure of $U_L(t,0)$ is then known.

Using the gauge transformed H, we want to study the Heisenberg evolution of π_μ and η_μ. We observe that it is the behavior of $\pi_\mu(t)$ and $\eta_\mu(t)$ instead of that of $p_\mu(t)$ and $x_\mu(t)$ that directly leads to the factorization of $U(t,t_0)$. We have

$$\dot{\pi}_\mu = \omega\epsilon_{\mu\nu}\pi_\mu - \frac{qB}{2c}\epsilon_{\mu\nu}\dot{R}_\mu(t), \quad \dot{\eta}_\mu = -\frac{qB}{2c}\epsilon_{\mu\nu}\dot{R}_\mu(t), \tag{13}$$

where $\omega = \frac{qB}{mc}$, or

$$\dot{\pi} = -i\omega\pi + i\frac{qB}{2c}\dot{R}(t), \quad \dot{\eta}_\mu = -\frac{qB}{2c}\epsilon_{\mu\nu}\dot{R}_\mu(t), \tag{14}$$

where

$$\pi = \pi_1 + i\pi_2, \quad R(t) = R_1(t) + iR_2(t). \tag{15}$$

The solution to the Heisenberg equations can then be expressed as

$$\pi(t) = \pi(0)e^{-i\omega t} + i\frac{qB}{2c}e^{-i\omega t}\int_0^t e^{i\omega s}\frac{d}{ds}R(s)ds, \tag{16}$$

$$\eta_\mu(t) = \eta_\mu(0) - \frac{qB}{2c}\epsilon_{\mu\nu}(R_\nu(t) - R_\nu(0)). \tag{17}$$

It is very clear that the homogeneous terms in the expressions for $\pi(t)$ and $\eta_\mu(t)$ can be generated by the usual dynamical operator $D(t) = \exp(-iH_L(0)t/\hbar)$. To produce the extra terms in the expression for $\pi(t)$, and $\eta_\mu(t)$, respectively using an operator $W(t)$, such that $D(t)W(t)$ recovers the whole solution, it suffices for $W(t)$ to satisfy:

$$W^\dagger(t)\pi(0)W(t) = \pi(0) + i\frac{qB}{2c}\int_0^t e^{i\omega s}\frac{d}{ds}R(s)ds, \tag{18}$$

$$W^\dagger(t)\eta_\mu(0)W(t) = \eta_\mu(0) - \frac{qB}{2c}\epsilon_{\mu\nu}(R_\nu(t) - R_\nu(0)). \tag{19}$$

In view of the commutation relations (1), which imply $[\pi, \pi^\dagger] = 2\hbar qB/c$, and from the formula $\exp(-B)A\exp(B) = A + [A, B]$ with the condition that $[A, B]$ commutes with A and B, it is clear that $W(t)$ can be chosen to be the product of two mutually commuting operators, generated by $(1, \pi(0), \pi^\dagger(0))$ and $(1, \eta_1(0), \eta_2(0))$ respectively. Each of theses operators produces a translation for either $\pi(0)$ or $\eta_\mu(0)$ while leaving the other unchanged. Writing $W(t)$ as $W(t) = K(t)M(t)$, we can make the following choice for $K(t)$ and $M(t)$,

$$K(t) = T\exp\Big(i\frac{\pi^\dagger(0)}{4\hbar}\int_0^t e^{i\omega s}\frac{d}{ds}R(s)ds + i\frac{\pi(0)}{4\hbar}\int_0^t e^{-i\omega s}\frac{d}{ds}R^*(s)ds\Big), \tag{20}$$

$$M(t) = P\exp\big(-i\hbar^{-1}\eta_\mu(0)\frac{R_\mu(t) - R_\mu(0)}{2}\big), \tag{21}$$

where $T\exp$ stands for time-ordered exponential. It's different from the direct exponential by a numerical phase factor only, similar to the path-ordered exponential. Therefore it can be directly checked that $D(t)K(t)M(t)$ recovers the solutions to the Heisenberg equations.

To verify that $D(t)K(t)M(t)$ not only recovers the solutions to the Heisenberg equations for π and η_μ, but in fact is the time evolution operator corresponding to H, we now verify that it satisfies the Schrödinger equation. Note that $M(t)$ commutes with both $D(t)$ and $K(t)$, so we have

$$i\hbar\frac{\partial}{\partial t}\big(D(t)K(t)M(t)\big) = i\hbar\big[\frac{\partial}{\partial t}\big(D(t)M(t)\big)\big]K(t) + i\hbar M(t)D(t)\frac{\partial}{\partial t}K(t). \tag{22}$$

It is straightforward that

$$i\hbar\big[\frac{\partial}{\partial t}\big(D(t)M(t)\big)\big]K(t) = \big(H_0(0) + \eta_\mu\dot{R}_\mu(t)/2\big)D(t)K(t)M(t). \tag{23}$$

To calculate $i\hbar M(t)D(t)\frac{\partial}{\partial t}K(t)$, first observe that

$$D(t)\pi(0)D^\dagger(t) = D^\dagger(-t)\pi(0)D(-t) = \pi(0)e^{i\omega t}, \tag{24}$$

$$D(t)\pi^\dagger(0)D^\dagger(t) = \big(D(t)\pi(0)D^\dagger(t)\big)^\dagger = \pi^\dagger(0)e^{-i\omega t}. \tag{25}$$

Therefore

$$
\begin{aligned}
i\hbar M(t)D(t)\frac{\partial}{\partial t}K(t) &= \big(-\pi^\dagger(0)\dot{R}(t)/4 - \pi(0)\dot{R}^*(t)/4\big)D(t)K(t)M(t), \\
&= -\frac{1}{2}\big(\pi_1(0)R_1(t) + \pi_2(0)R_2(t)\big)D(t)K(t)M(t). \quad (26)
\end{aligned}
$$

Combining terms and from the definitions of π_μ and η_μ, we now have

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\big(D(t)K(t)M(t)\big) &= \big(H_L(0) + \frac{qB}{2c}x_1\dot{R}_2 - \frac{qB}{2c}x_2\dot{R}_1\big)D(t)K(t)M(t), \\
&= H\big(D(t)K(t)M(t)\big). \quad (27)
\end{aligned}
$$

Therefore we conclude that the time evolution operator corresponding to H is

$$
U(t,0) = D(t)K(t)M(t) = M(t)D(t)K(t). \quad (28)
$$

And the time evolution operator corresponding to the original Hamiltonian H_L is

$$
U_L(t,0) = \exp[-i\frac{q}{\hbar c}\chi(\mathbf{x},\mathbf{R}(t))]M(t)D(t)K(t) \quad (29)
$$

Noteworthy is the explicit construction of the operator $K(t)$ that depends on the rate of change of the parameter $\mathbf{R}(t)$. It approaches the identity operator in the adiabatic limit of $\dot{R}_\mu(t) \to 0$, though the formula is valid for a general variation of the parameter, not necessarily adiabatically. $M(t)$ on the other hand is a geometric operator. It is determined by the path C traversed by $\mathbf{d}(t) = (\mathbf{R}(t) - \mathbf{R}(0))/2$, and recovers a geometric phase ($\beta(C(\mathbf{d}))$ in equation (3)) for a closed path when acting on an eigenstate.

What about nonadiabatic transitions? For a general variation of the parameter, we have to resort to the general expression for $K(t)$. For a slow variation of the parameter $\mathbf{R}(t)$, say $\mathbf{R}(t) = \mathbf{R}(\epsilon t)$, where $T = \frac{1}{\epsilon}$ is the duration of the adiabatic process, perturbative treatment is possible. The oscillating kernels in the integrals in the expression for $K(t)$ make sure that the transition probability is of the order ϵ^2 for the entire duration T of the adiabatic process. Because $\pi^\dagger(0)$ and $\pi(0)$ have the meaning of being proportional to the creation and annihilation operators on the energy eigenstates, the transition probability should be of the order of $n^2\epsilon^2/\omega^2$, during the entire adiabatic process $0 \le t \le T$, where n is the energy quantum number of a Landau level, $E_n = \hbar\omega(n + 1/2)$. Therefore nonadiabatic transition rates are energy level dependent and increase as n^2.

In conclusion, our construction of the time evolution operator $U_L(t,0)$ can be characterized as seeing the magnetic translation of a charged particle accompanied by nonadiabatic corrections through a gauge transformation. It provides an example of how the quantum adiabatic theorem is realized when infinitely degenerate energy levels are involved. Since the factorization is valid for a general time variation, it can be employed to study the evolution of all kinds of initial states of the system and their geometric phases, not only adiabatic evolutions of initial eigenstates.

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